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MEMORANDUM FOR PRS (In-House Publication)

FROM: PROI (STINFO) 29 April 2002

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-TP-2002-090** Jerry Boatz (PRSP) et al., "Simulations of Energetic Materials for Rocket Propulsion: Obtaining More 'Bang for the Buck'"

DoD HPC Success Story Publication **(Statement A)**
(Deadline: 15 May 2002)

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PHILIP A. KESSEL Date
Technical Advisor
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Title: Simulations of Energetic Materials for Rocket Propulsion: Obtaining More "Bang for the Buck"

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HPC Resource Environments: SGI Origin 2000 at ARL, Cray T3E at NAVO, IBM SP/P3 at ASC.

Powderized aluminum has long been used as an energetic ingredient in rocket propellant formulations, comprising approximately 15-20% of some conventional ammonium perchlorate solid propellant formulations. However, the performance of aluminum is reduced by the rapid formation of an aluminum oxide overcoat on aluminum particles prior to combustion, which also inhibits efficient burning. Furthermore, formation of the oxide overcoat severely reduces the potential advantages of using high surface-to-volume-ratio ultrafine aluminum particles, which would otherwise have highly desirable properties such as enhanced burn rates.

In order to inhibit the rapid formation of an oxide overcoat on the ultrafine aluminum particles without simultaneously degrading performance, it has been proposed to coat the aluminum particles with an energetic material such as HMX. One of the objectives of this challenge project is to characterize the interactions between energetic compounds such as HMX and aluminum surfaces in order to understand, at an atomic level, the chemistry at the metal-molecule interface. Specifically, ab initio quantum chemical calculations are used to determine if HMX and/or other

classes of energetic materials will effectively inhibit the formation of an oxide overcoat on the surface of aluminum.

Conventional techniques for determining the feasibility of new ideas such as this have relied heavily on costly and time-consuming experimental synthesis and testing. However, the availability of HPC resources has significantly lessened the need for these empirical approaches by enabling the application of reliable high-level quantum chemical calculations to address complex issues such as the nature of the interactions between energetic materials and metallic surfaces. A key advantage of using HPC in this regard is the ability to efficiently "screen" a variety of energetic materials as potential metallic coatings and focus subsequent experimental efforts on the subset of only the promising candidates.

Spin-polarized GGA density functional theory, using ultrasoft Vanderbilt-type pseudopotentials and the PW91 exchange-correlation functional in a plane-wave basis, has been used to characterize the interactions between the energetic molecules nitromethane (NM), HMX, and FOX-7 and the aluminum (111) surface. Two different models have been used to approximate the (111) surface of aluminum: a $(\sqrt{7}x\sqrt{7})$ R19.1° slab model with four layers (28 aluminum atoms) used for NM and a four-layer (3x3) slab (36 atoms) for the larger molecules (HMX and FOX-7). All calculations were performed using the VASP code.

Preliminary predictions of the interactions between the energetic molecules nitromethane (NM), HMX and FOX7 have indicated a common propensity for oxidation of the aluminum surface by the oxygen-rich nitro groups (NO2) present in these molecules. Dissociation of the nitro groups and formation of strong Al-O bonds appears to be a common mechanism for these molecules. These results suggest that nitro-containing energetic compounds are not likely to be effective coating materials for preventing rapid oxidation of aluminum.

Future work will extend this set of investigations to first principles density functional theory calculations of the interactions of several ionic systems such as ammonium nitrate or ammonium dinitramide with an Al surface. In these investigations, key reaction pathways of these energetic salts on an aluminum surface will be computed. We will furthermore attempt to understand the type of chemical processes that can take place at the interface of aluminum hydrides with different classes of energetic materials. In this case we will focus on the case of ammonium nitrate and RDX crystals where the detonation properties are significantly affected by the interaction with aluminum hydrides.

Primary CTA: CCM

Scientific visualization: Construction of the initial atomic configurations for crystals, surfaces and gas-solid systems has been performed using the Crystal and Surface Builders modules available in Cerius2 package. Graphical visualization of the optimized atomic configurations has been done using the C2 Visualizer package also available on Cerius2 platform.

References: (1) J.A. Boatz, D.C. Sorescu, and D.L. Thompson, "Computational Studies of Advanced Materials", Arctic Region Supercomputing Center Technology Panel, University of Alaska-Fairbanks, 12-14 March 2002; (2) D. C. Sorescu, J. A. Boatz, and D. L. Thompson,

"Classical and Quantum Mechanical Studies of Crystalline FOX-7 (1,1-diamino-2,2-dinitroethylene)", J. Phys. Chem. A **105**, 5010-5021 (2001). (3) Cerius2 is a simulation and modeling environment offering a broad range of application modules available from Accelrys company.

Figure Caption: Initial (left) and final (right) configurations of an HMX molecule on an aluminum (111) surface. In the final configuration, one of the oxygen atoms is bonded to two surface aluminum atoms and is completely dissociated from the initial NO_2 group. The other oxygen atom also forms a bond with aluminum but remains bonded to the nitrogen atom in the original NO_2 group.

Acronyms:

NM	Nitromethane (CNO_2H_3)
HMX	$C_4N_8O_8H_8$, a cyclic nitramine
FOX-7	1,1-diamino-2,2-dinitroethylene ($C_2N_4O_4H_4$)
VASP	Vienna Ab Initio Simulation Package
GGA	Generalized gradient approximation
PW91	Perdew-Wang exchange-correlation functional.